

# Kondo Effect and Non-Fermi Liquid Behavior in Dirac Materials

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Work supported by



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## Kondo Effect in Dirac Materials

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## Effect of Spin-orbit coupling on impurity bound states in superconductors

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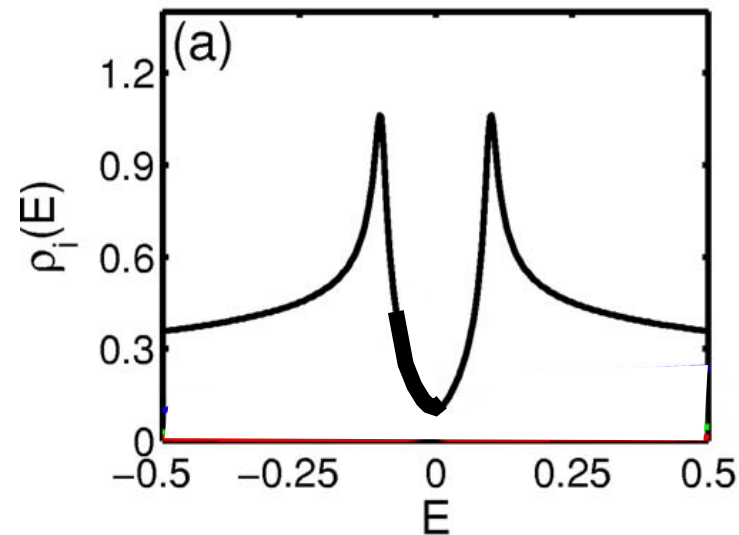


Microsoft Research, Station Q

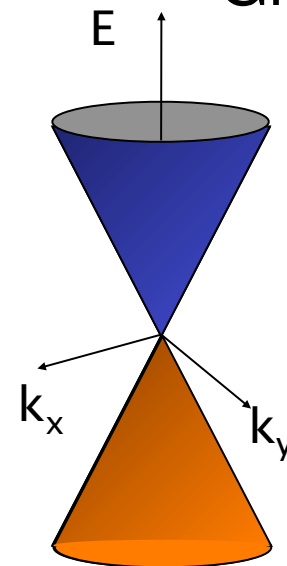
# Dirac Materials

## 2D Dirac Materials

d-wave  
superconductors

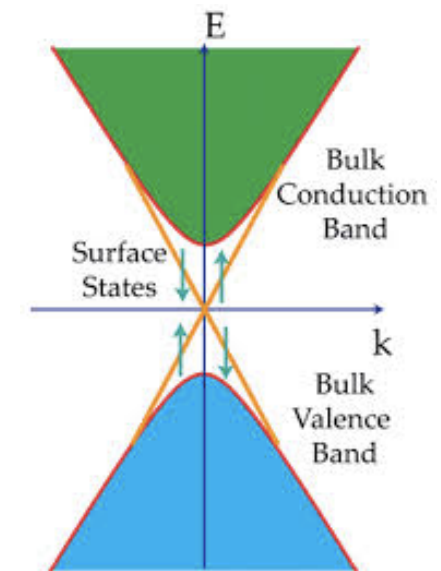


Graphene



$$\mathcal{H} = v_F \mathbf{p} \cdot \boldsymbol{\sigma}$$

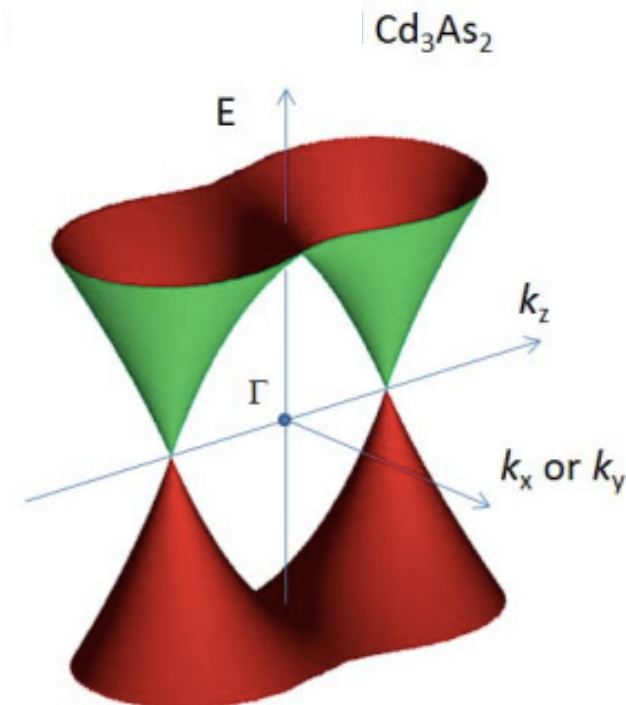
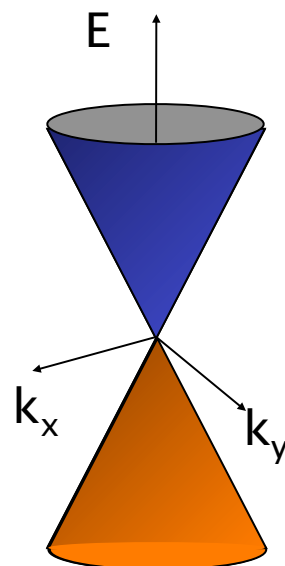
3D TI's surfaces



## 3D Dirac Materials

3D Graphene and Weyl Semimetals

$$\mathcal{H} = v_F \mathbf{p} \cdot \boldsymbol{\sigma}$$

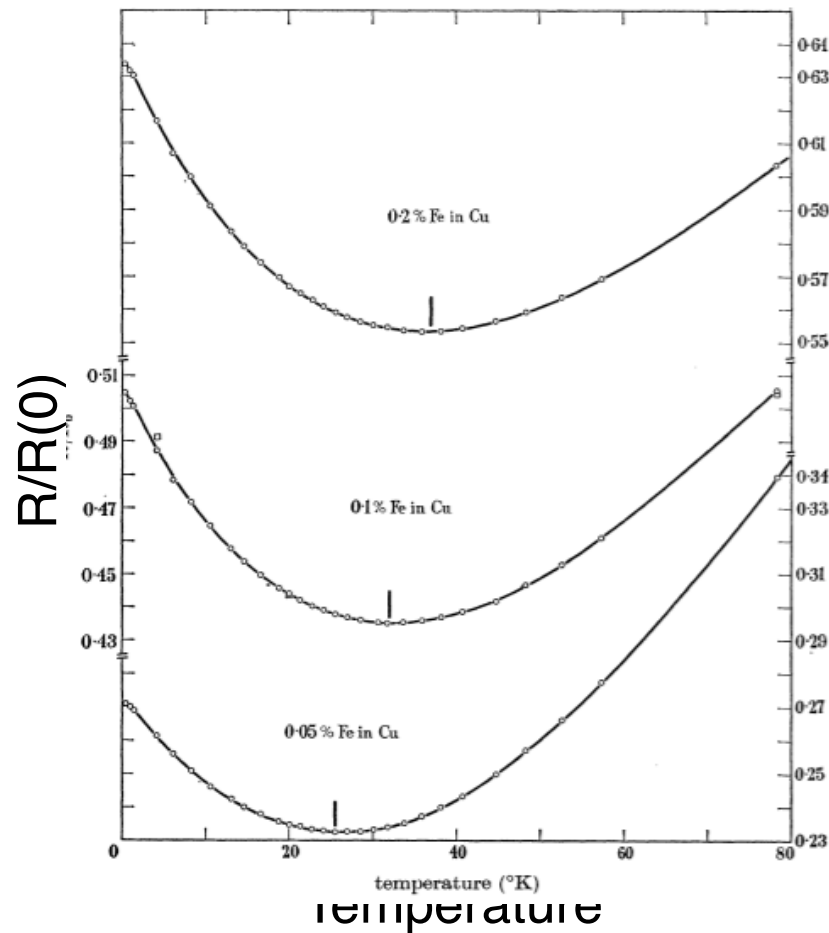


# Kondo Effect

$$\rho(T) = \rho_0 + bT^5 - a \ln(T)$$

There is a crossover temperature,  $T_K$ , below which the coupling between the conduction electrons and the *dynamical* magnetic impurity grows non-perturbatively

$T < T_K$  Formation of a many-body singlet



J. P. Franck, F. D. Manchester and Douglas L. Martin, Proc. Royal Society of London 1961

For standard case

$$T_K = D e^{-\frac{1}{J N(0)}}$$

$$N(0) \propto \epsilon^\alpha$$

**Pseudogap Kondo problem**

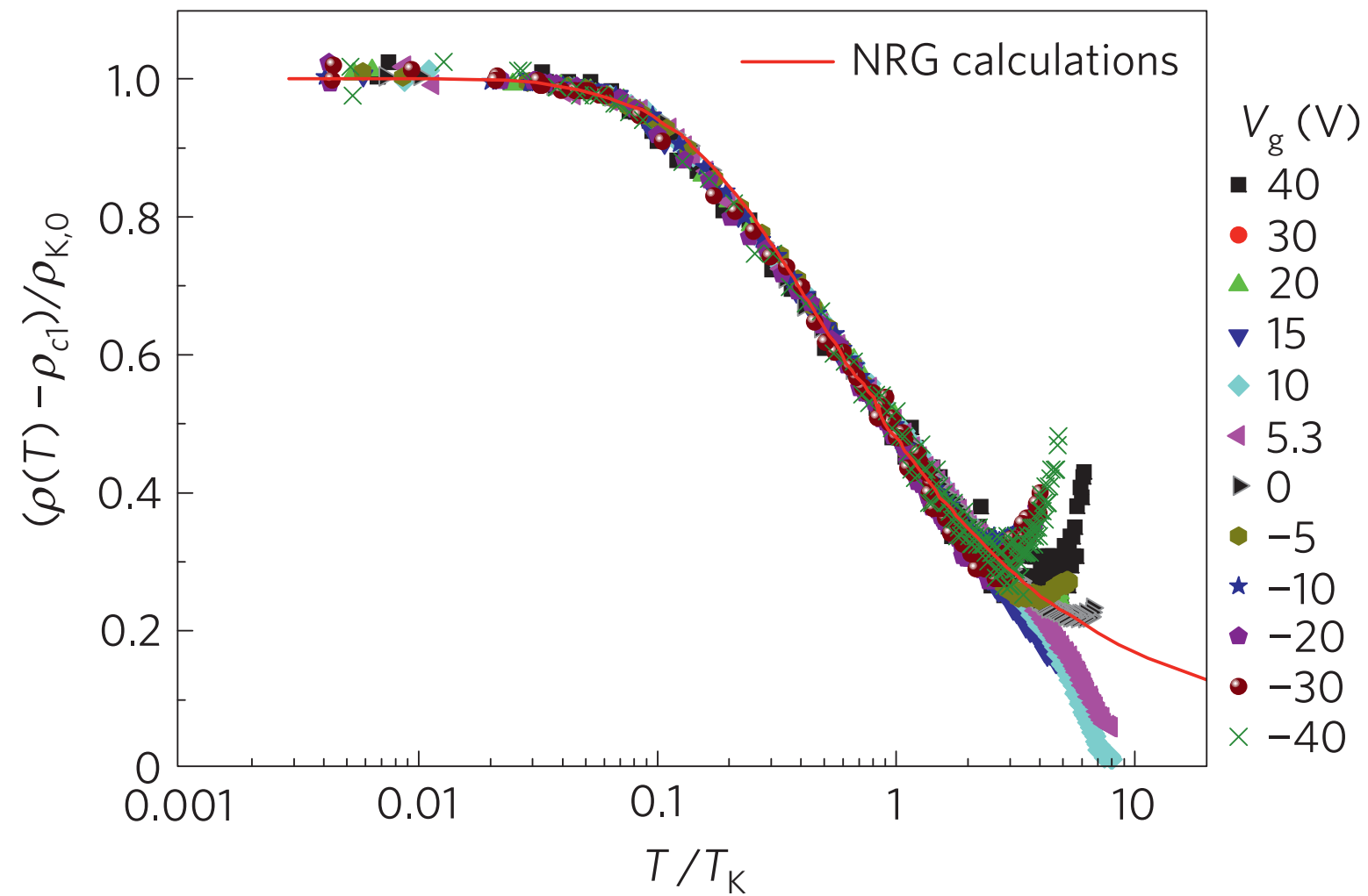


Withoff and Fradkin(1990),  
Ingersent (1996), ... A.V.  
Balatsky et al. RMP (2006),  
Fritz and Vojta Reports on  
Progress in Physics (2013)



# Experimental evidence

Graphene



Jian-Hao Chen et al. Nat. Phys. (2011)

# Theoretical approach

$$H = H_{DM} + H_{\text{imp}}$$

$$H_{DM} = \hbar v_F \hat{c}_{\mathbf{k}\sigma}^\dagger (\mathbf{k} \cdot \boldsymbol{\tau}_{\sigma\sigma'} - \mu) \hat{c}_{\mathbf{k}\sigma'}$$

$$H_{\text{imp}} = J \sum_{\mathbf{r}, \mathbf{R}} \hat{c}_{\mathbf{r}\sigma}^\dagger \boldsymbol{\tau}_{\sigma\sigma'} \hat{c}_{\mathbf{r}\sigma'} \cdot \mathbf{S} \delta(\mathbf{r} - \mathbf{R})$$

## Large-N expansion

$\mathbf{S}$  is expressed in terms of auxiliary fermionic operators “f” satisfying the constrain

$$n_f = \sum_{\sigma} \hat{f}_{\sigma}^\dagger \hat{f}_{\sigma} = 1. \quad \text{Then}$$

$$H_{\text{imp}} = J \sum_{\mathbf{k}, \mathbf{k}', \sigma} \hat{c}_{\mathbf{k}\sigma}^\dagger \hat{c}_{\mathbf{k}'\sigma'} \hat{f}_{\sigma'}^\dagger \hat{f}_{\sigma}$$

The interaction is decoupled via the mean-field

$$s \sim \sum_{\mathbf{k}, \sigma} \langle \hat{f}_{\sigma}^\dagger \hat{c}_{\mathbf{k}\sigma} \rangle$$

And the constrain on  $n_f$  is enforced via a Lagrange multiplier  $\mu_f$

## Determination of $T_K$

The field “s” and the Lagrange multiplier are obtained via the self-consistent equations:

$$\int_{-D-\mu}^{D-\mu} d\varepsilon \frac{n_F(\varepsilon)(\varepsilon - \mu_f)\mathcal{N}(\varepsilon + \mu)}{(\varepsilon - \mu_f)^2 + (\pi |s|^2 \mathcal{N}(\varepsilon + \mu)/2)^2} = -\frac{1}{J}$$

$$\int_{-D-\mu}^{D-\mu} d\varepsilon \frac{n_F(\varepsilon) |s|^2 \mathcal{N}(\varepsilon + \mu)}{(\varepsilon - \mu_f)^2 + (\pi |s|^2 \mathcal{N}(\varepsilon + \mu)/2)^2} = 1$$

We identify  $T_K$  as the highest  $T$   
for which the two self-consistent equations admit a solution

# Scalings for $T_K$

At the Dirac point  $\mu = 0$

**3D**

$$T_K = D \frac{\sqrt{3}}{\pi} \sqrt{1 - \frac{2}{\mathcal{N}(D)J}}$$

$$J_{cr} = 2/\mathcal{N}(D)$$

**2D**

$$T_K = \frac{D}{\ln(4)} \left[ 1 - \frac{1}{\mathcal{N}(D)J} \right]$$

$$J_{cr} = 1/\mathcal{N}(D)$$

Withoff and Fradkin PRL (1990), Sengupta and Baskaran PRB (2008), E. Orignac and S. Burdin PRB (2013), C. Gonzalez-Buxton and K. Ingersent PRB (1998)

Away from Dirac point  $\mu \neq 0$

In the limit  $k_B T_K \ll \mu \ll D$  and  $J \lesssim J_c$

**3D**

$$T_K = D \exp \left[ \frac{1 - 2/(J\mathcal{N}(D))}{2\mu^2/D^2} \right]$$

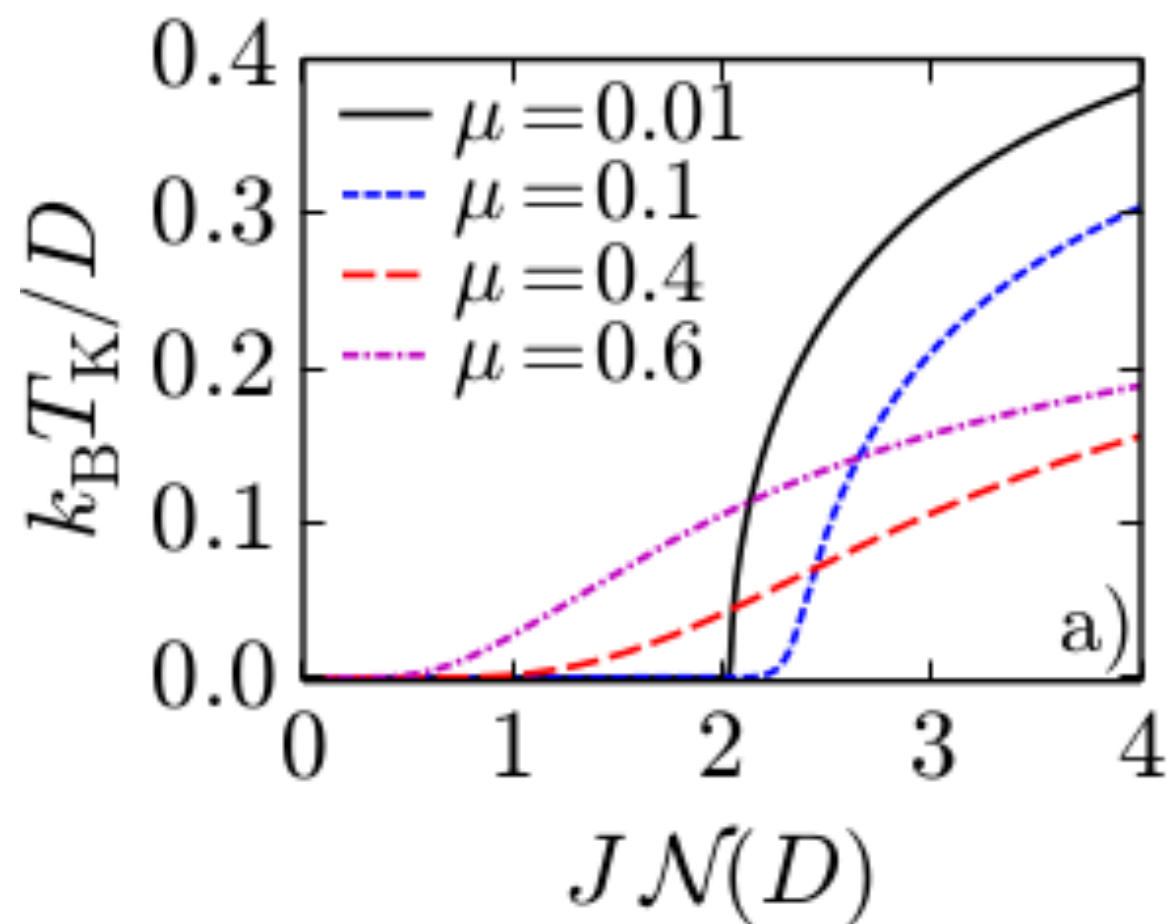
**2D**

$$T_K = \kappa(\mu) \exp \left[ \frac{1 - 1/(\mathcal{N}(D)J)}{|\mu/D|} \right]$$

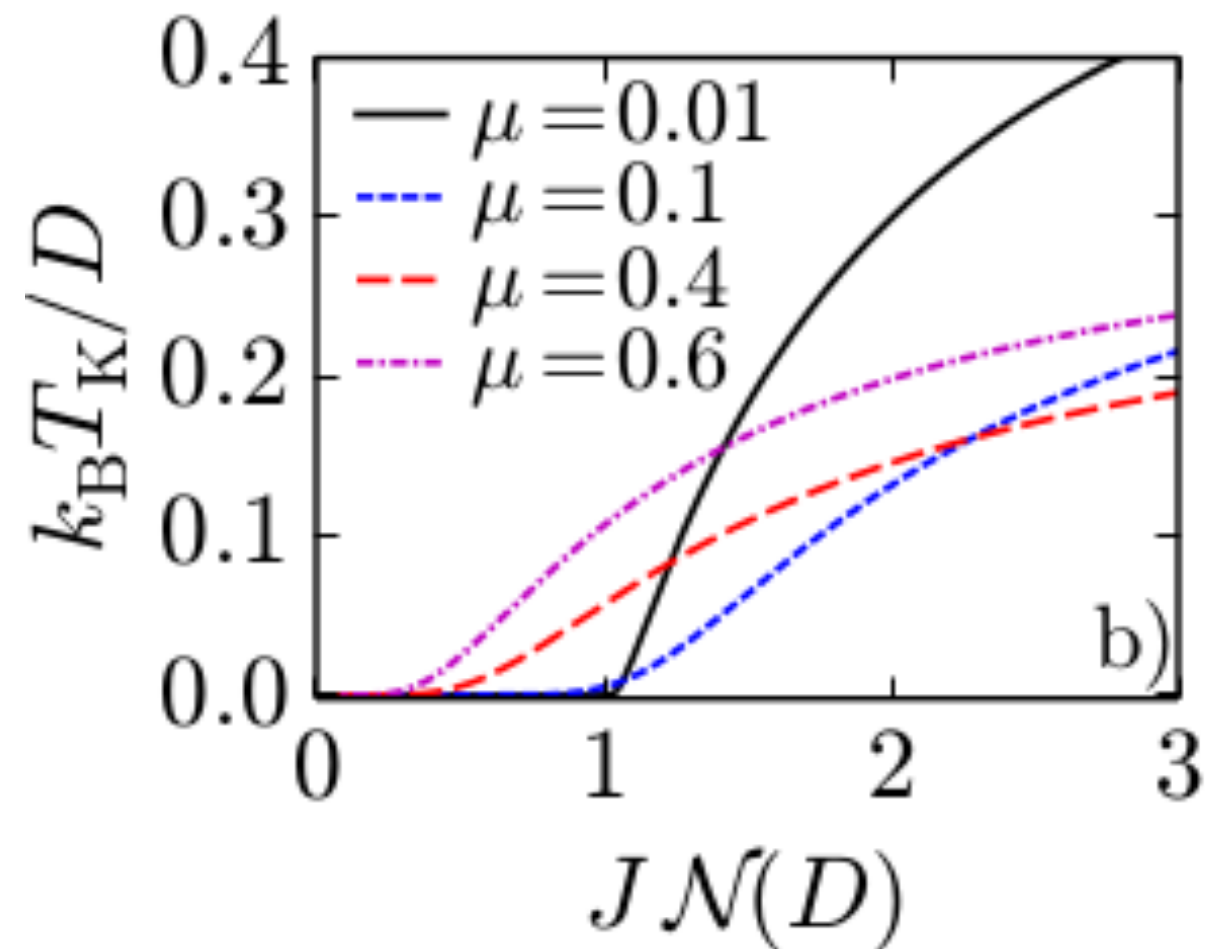
where  $\kappa(\mu) = \mu^2/D$  [ $\kappa(\mu) = D$ ] for  $\mu > 0$  [ $\mu < 0$ ].

## Scalings for $T_K$ : general case

**3D**



**2D**





# Kondo resistivity: $\rho_K$

In the limit  $T=0$

**3D**

$$\rho_K(T=0) = \frac{h}{e^2} \left( \frac{32g_s}{3\pi^2 N_w^2} \right)^{1/3} \frac{n_{\text{imp}}}{n^{4/3}}$$

Same scaling as for the case of non magnetic long-range scatterers

AA Burkov, MD Hook, L. Balents PRB (2011)

**2D**

$$\rho_K = \frac{h}{e^2} \frac{4}{\pi N_w} \frac{n_{\text{imp}}}{n}$$

P.S. Cornaglia et al, PRL (2009)

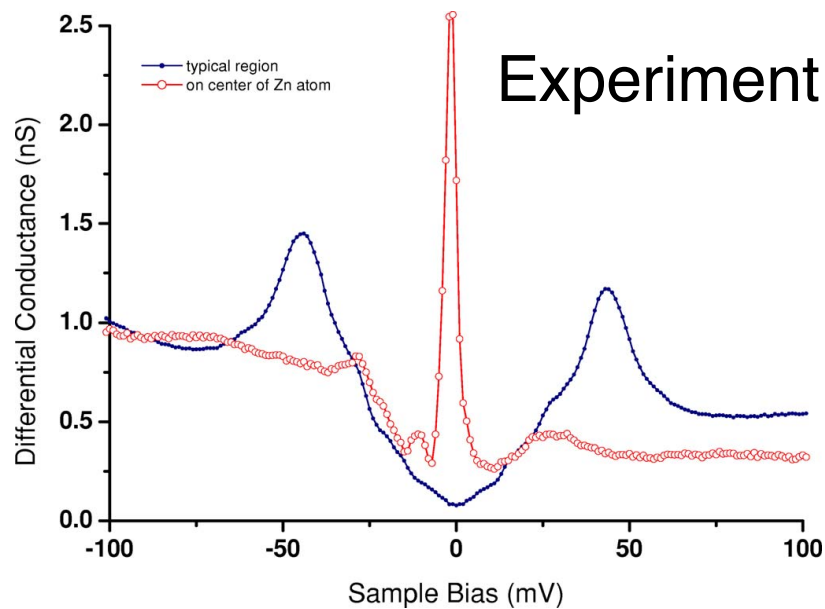
At finite  $T$

$$\rho(T) \simeq -\rho_0 \frac{\pi^2}{2} [J\nu(\mu)]^3 S(S+1) \ln \left( \frac{k_B T}{D} \right)$$

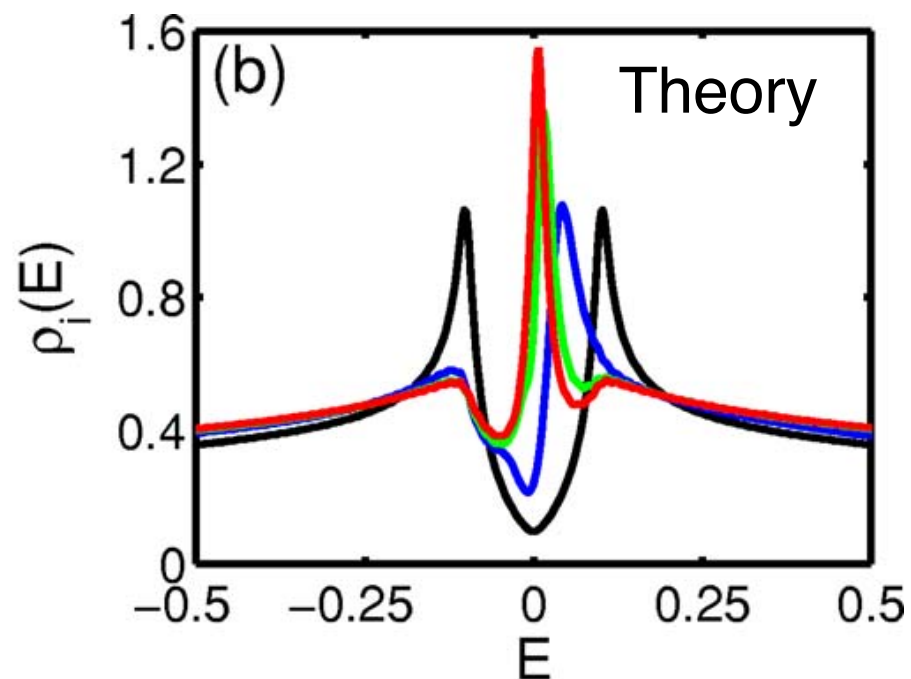
# Interplay of scalar and magnetic potential

$$H_{\text{imp}} = U \sum_{\mathbf{r}, \mathbf{R}} \hat{c}_{\mathbf{r}\sigma}^\dagger \hat{c}_{\mathbf{r}\sigma} \delta(\mathbf{r} - \mathbf{R}) + J \sum_{\mathbf{r}, \mathbf{R}} \hat{c}_{\mathbf{r}\sigma}^\dagger \boldsymbol{\tau}_{\sigma\sigma'} \hat{c}_{\mathbf{r}\sigma'} \cdot \mathbf{S} \delta(\mathbf{r} - \mathbf{R})$$

d-wave superconductors



Pan, S. H., E. W. Hudson, K. M. Lang, H. Eisaki, S. Uchida, and J. C. Davis, 2000, Nature (London) **403**, 746.



Buchholtz and Zwicknagl (1981),  
Stamp (1987), Balatsky *et al.* (1995),  
Salkola *et al.* (1996, 1997)

The scalar part of the impurity potential  
modifies the LDOS

It modifies  $T_K$  uniformly across the sample

$T_K$  is uniform across the sample  
and well defined

If the short range scalar potential is  
due to *other* impurities removed  
from the magnetic impurity it has  
little consequence.

## Long-range disorder

Charge impurities are a common source of disorder. However they can often be treated as short range disorder. Things are different in most Dirac materials

- Linear dispersion  $\Rightarrow$  vanishing DOS close to Dirac points  
 $\Rightarrow$  poor screening of the disorder due to charge impurities

The disorder is renormalized but  
retains its long-range character

- Charge impurities therefore cause strong, long-range, *density* inhomogeneities close to Dirac point
- Linear dispersion

Strong, long-range, *density inhomogeneities*



Strong, long-range, inhomogeneities of the DOS

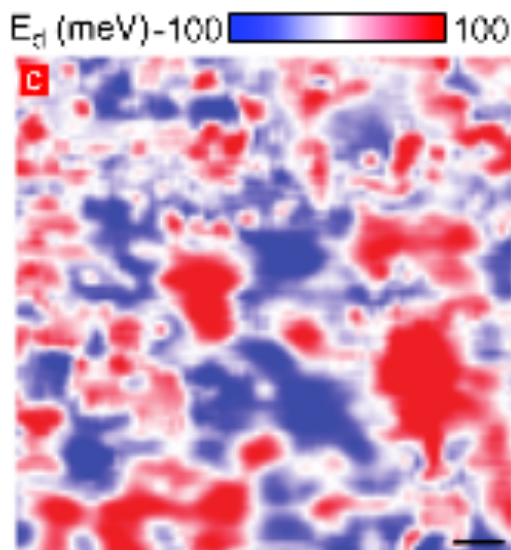
# Interplay of scalar and magnetic potential: long-range scalar potential

Not important in  
superconductors:  
well screened

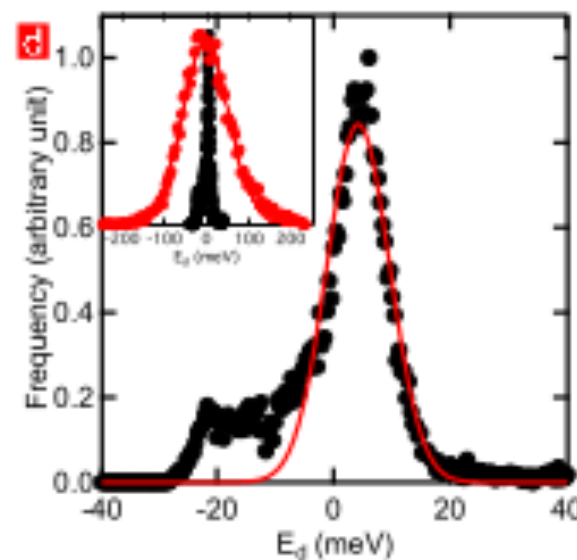
Charge impurities

In non-superconducting Dirac materials, due to vanishing DOS they induce strong, long-range, carrier density inhomogeneities

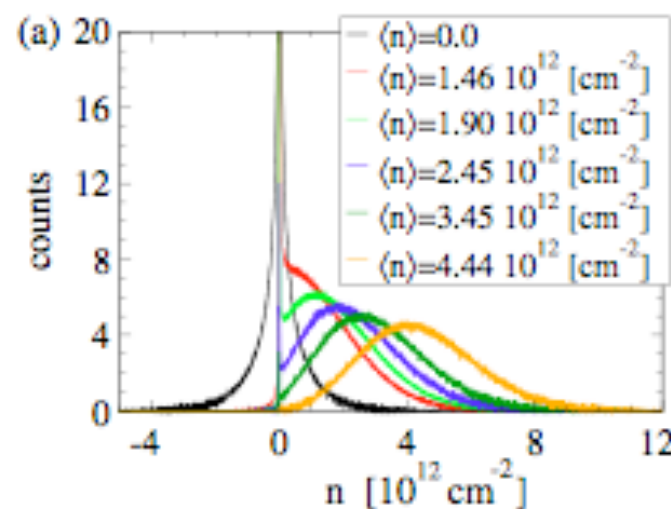
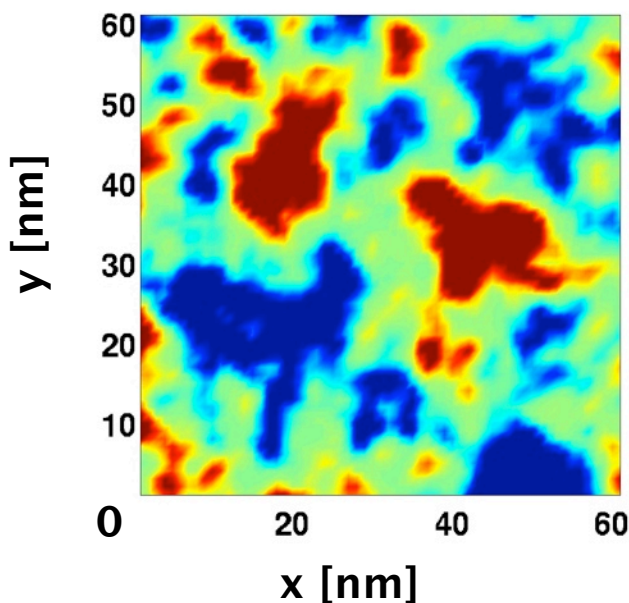
**Experiment**



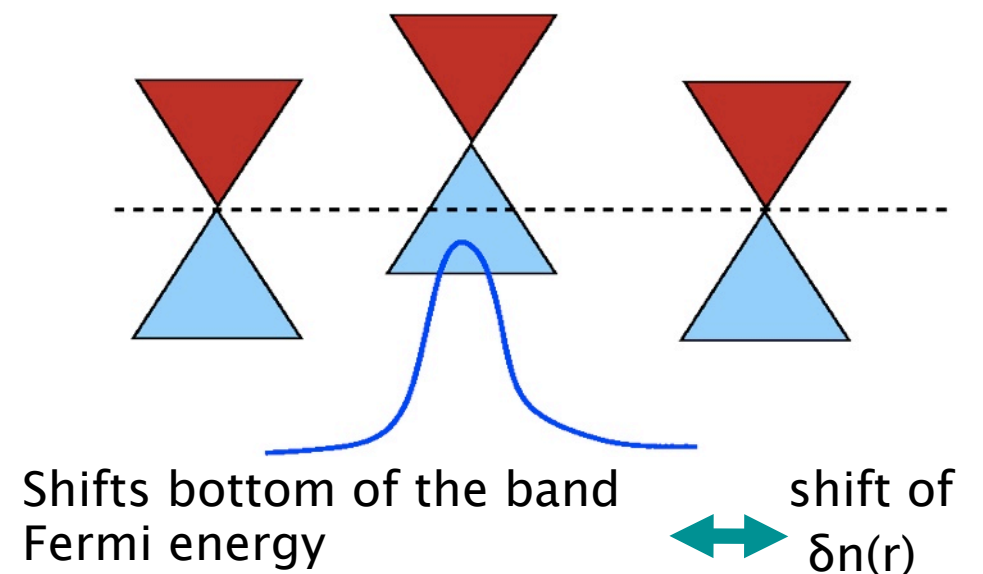
J. Xue et al. Nat. Mat. (2011)



**Theory**



ER, S. Das Sarma, PRL. (2008)



**2D**

**LDOS  $\sim n$**

**3D**

**LDOS  $\sim n^{2/3}$**

**Fluctuations of  $n$   
imply fluctuations of LDOS**

J. Martin et al. Nat Phys. (2008)  
Y. Zhang et al. Nat. Phys. (2009)

# Effect of long-range scalar disorder

For simplicity we assume a Gaussian distribution for the density probability

$$P_n(n) = \exp \left[ - (n - \bar{n})^2 / (2\sigma_n^2) \right] / (\sqrt{2\pi}\sigma_n).$$

Using the relation between  $T_K$  and  $\mu$  and the fact that

$$\text{in 3D: } \mu \sim n^{1/3} \quad \text{in 2D: } |\mu| \sim n^{1/2}$$

**Instead of a single value of  $T_K$  we have a distribution of  $T_K$**

**3D**

$$P^{(3D)}(T_K) = \frac{3D^3}{8\sqrt{\pi}\sigma_\mu^3 T_K} \left[ \frac{(1 - J_c/J)^3}{\ln^5(k_B T_K/D)} \right]^{1/2} \left[ e^{-\frac{(\mu^3 - \bar{\mu}^3)^2}{2\sigma_\mu^6}} + e^{-\frac{(\mu^3 + \bar{\mu}^3)^2}{2\sigma_\mu^6}} \right]$$

$$P^{(3D)} \propto \frac{1}{T_K [\ln(T_K)]^{5/2}}$$

**2D**

$$P^{(2D)}(T_K) = \frac{\sqrt{2}D^2}{\sqrt{\pi}\sigma_\mu^2 T_K} \frac{(1 - J_c/J)^2}{|\ln^3(k_B T_K/D)|} \left[ e^{-\frac{(\mu^2 - \bar{\mu}^2)^2}{2\sigma_\mu^4}} + e^{-\frac{(\mu^2 + \bar{\mu}^2)^2}{2\sigma_\mu^4}} \right]$$

$$P^{(2D)} \propto \frac{1}{T_K [\ln(T_K)]^3}$$

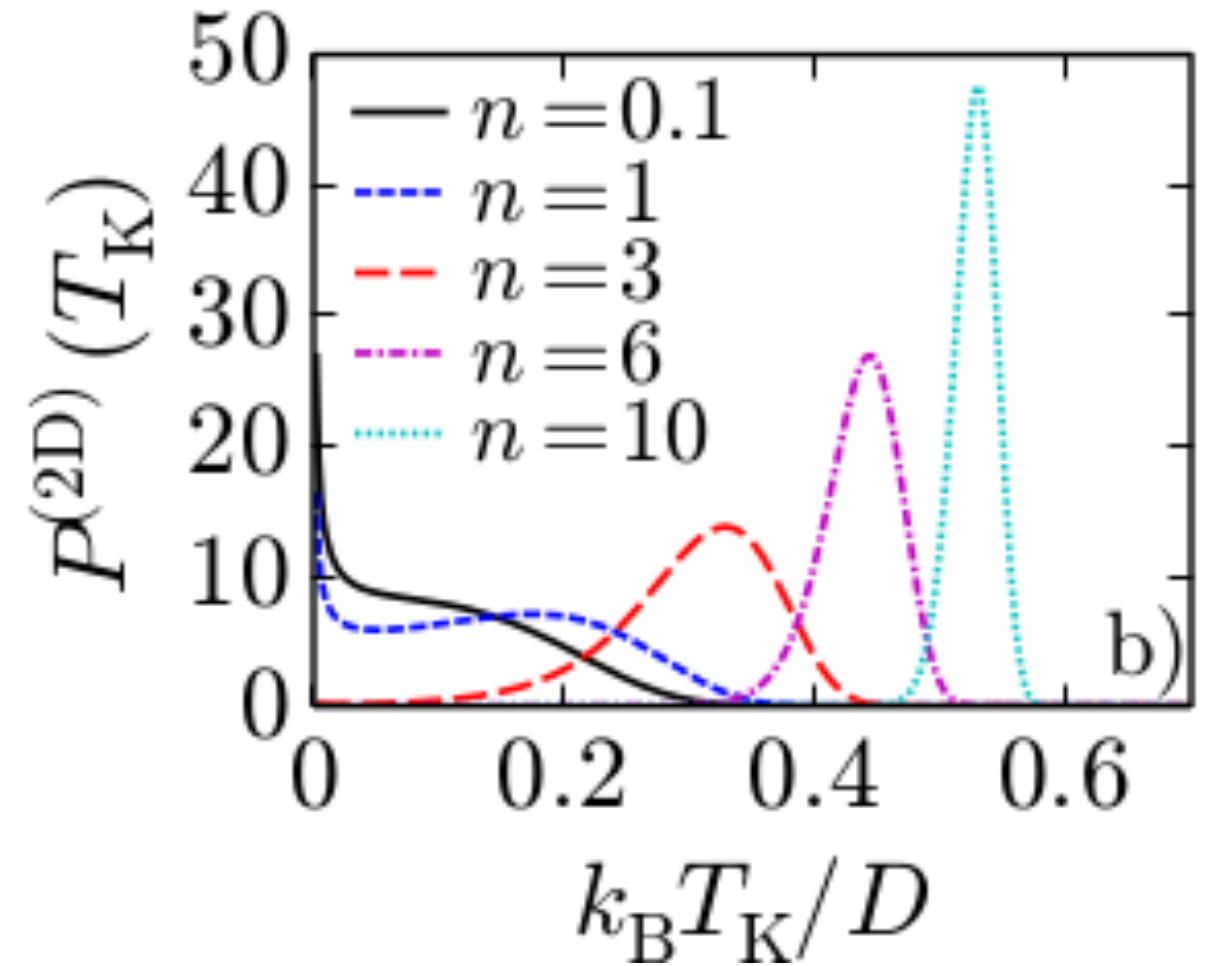
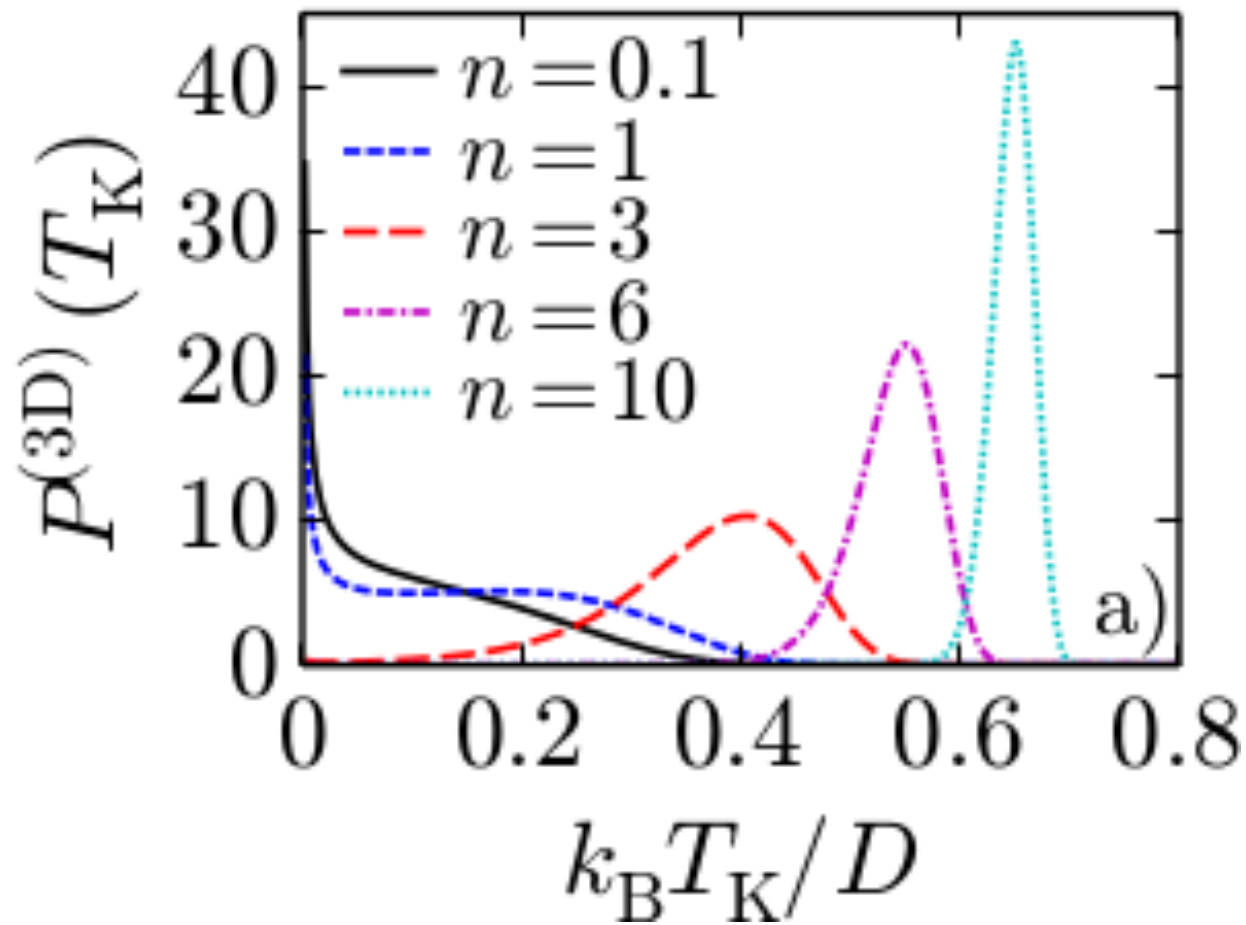
Agrees with scaling obtain from numerical results by V.G. Miranda et al PRB (2014)



# $P(T_K)$

3D

2D



For low  $T_K$  the scaling  
 $1/[T_K \ln^3(T_K)]$   
 very similar to  
 $1/(T_K^{0.8})$   
 obtained by fitting numerical results by V.G.  
 Miranda et al. PRB (2014)

# LDOS fluctuations close to MIT

Typically in materials other than Dirac materials is difficult to obtain strong, long-range fluctuations of the LDOS. A similar situation can be obtained close to a metal-insulator transition. In this case the probability distribution for the LDOS  $\rho$  is log-normal

$$P(\rho) = \frac{1}{\sqrt{4\pi u}} \frac{1}{\rho} \exp \left\{ -\frac{1}{4u} \ln^2 \left[ \frac{\rho}{\rho_0} e^u \right] \right\}.$$

I.V. Lerner, Phys. Lett. A (1988),  
B.L. Altshuler and V.N. Prigodin JETP (1987)

In this case we also get a singular distribution for  $T_K$

$$P(T_K) = (4\pi u)^{-1/2} \frac{1}{T_K \ln(\epsilon_F/T_K)} \exp \left\{ -\frac{1}{4u} \ln^2 [\rho_0 J e^{-u} \ln(\epsilon_F/T_K)] \right\}$$

V. Dobrosavlyevic, T.R. Kirkpatrick, G. Kotliar  
PRL (1992)

However:

- The conditions are difficult to achieve
- The effects are weaker than in Dirac Materials

## Free carriers even for $T \rightarrow 0$

Considering that

$$P^{(3D)} \propto \frac{1}{T_K [\ln(T_K)]^{5/2}}$$

$$P^{(2D)} \propto \frac{1}{T_K [\ln(T_K)]^3}$$

We see that at any is a considerable fraction of the sample for which  $T_K$  is very small



At any  $T$ , no matter how low, there is a significant fraction,  $n_{fr}$ , of carriers not **bound** to the impurities

We can obtain such fraction at temperature  $T$  by calculating the integral

$$n_{fr}(T) = \int_0^T dT_K P(T_K)$$

And we find, for  $T \rightarrow 0$

**3D**

$$n_{fr}(T) \propto |\ln(T)|^{-3/2} e^{-\bar{n}^2 / (2\sigma_n^2)}$$

**2D**

$$n_{fr}(T) \propto |\ln(T)|^{-2} e^{-\bar{n}^2 / (2\sigma_n^2)}$$

**Even for  $T \rightarrow 0$   $n_{fr}$  is significant**

# Non-Fermi liquid behavior

Consider the magnetic susceptibility. We have

$$\chi_m \propto \frac{n_{\text{fr}}(T)}{T}$$

And therefore we find:

**3D**

$$\chi_m \propto \frac{1}{T |\ln(T)|^{3/2}}$$

**2D**

$$\chi_m \propto \frac{1}{T |\ln(T)|^2}$$

**$\chi_m$  diverges for  $T \rightarrow 0$**

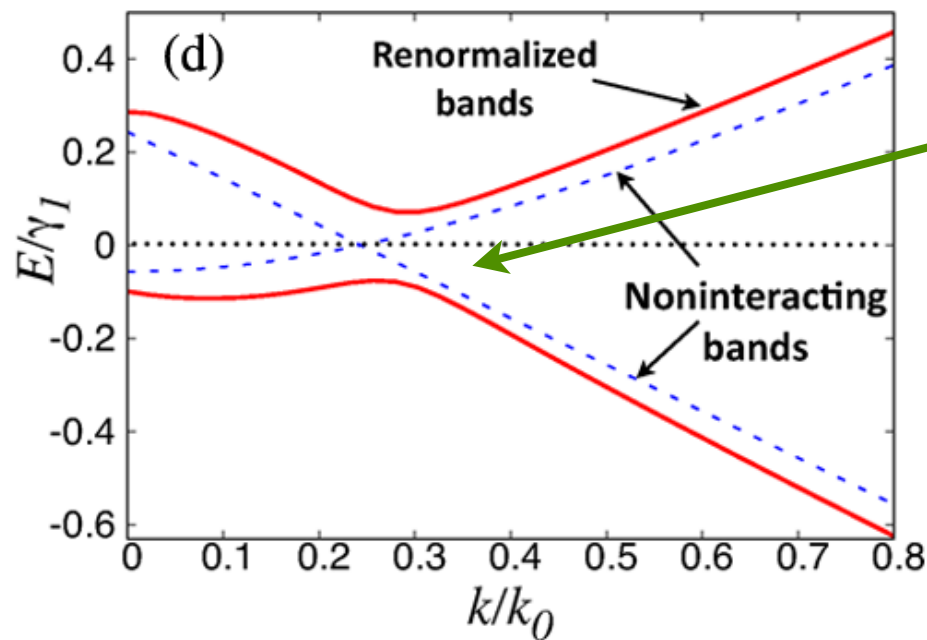


**Strong Non-Fermi-Liquid Behavior**

P. Nozieres (1974)

**$\chi_m$  also does not follow the Curie-Weiss law ( $1/T$ ) it diverges more slowly**

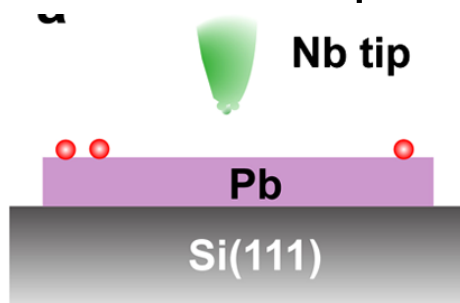
# Impurity-bound states in SCs with SOC: motivation



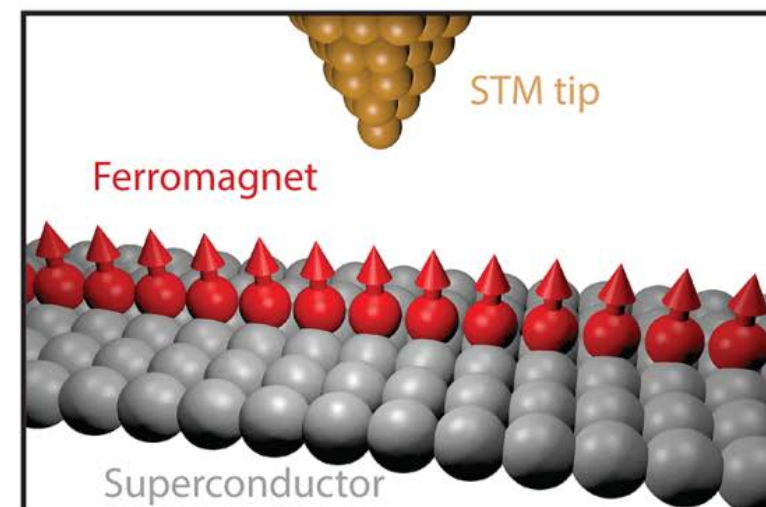
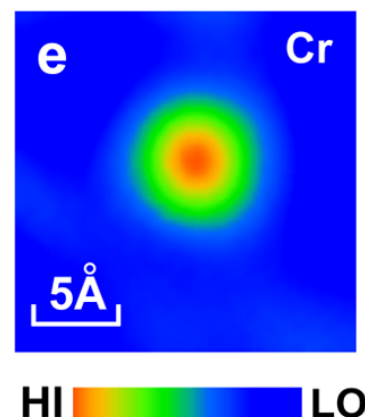
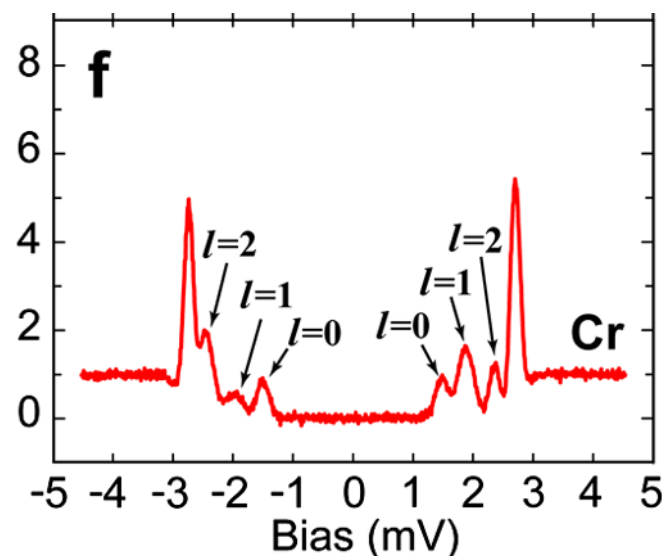
A magnetic impurity can create states with energies within the gap due to the superconducting pairing. These states are spatially bound to the impurity (Yu-Shiba-Rusinov). A chain of impurities can create a band of these states.

In the presence of SOC a FM chain on SC **with SOC** appears to have Majorana states at the ends

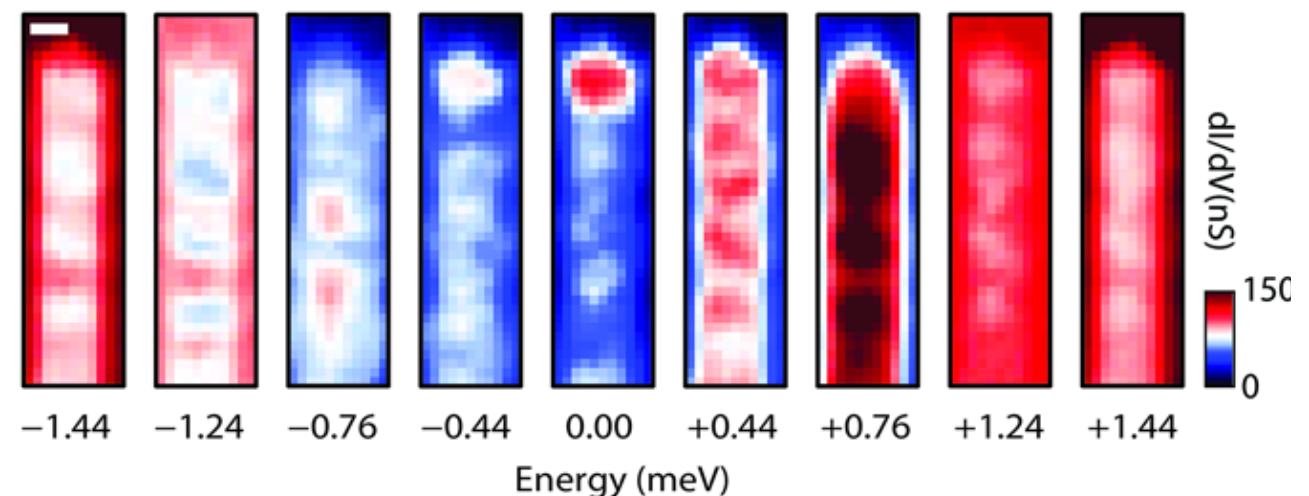
Measured using STM for isolated impurities



Shuai-Hua Ji et al.  
PRL (2008)

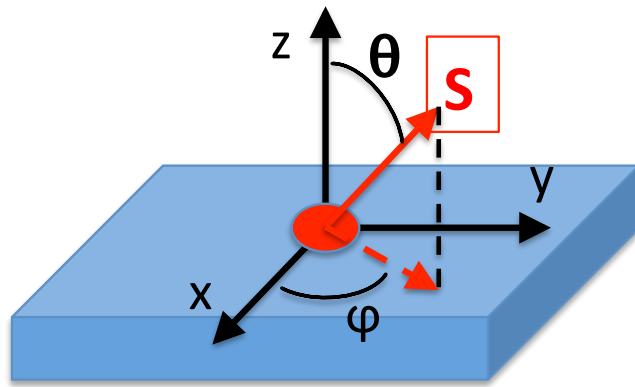


S. Nadj-Perge et al.  
Science (2014)





# Impurity-bound states in SCs with SOC: model



$$H = H_{SC} + H_{\text{imp}}$$

$$H_{SC} = \sum_{\mathbf{p}} \psi_{\mathbf{p}}^{\dagger} [\tau_z \otimes (\xi_{\mathbf{p}} + \underbrace{\alpha \mathbf{l}_{\mathbf{p}} \cdot \boldsymbol{\sigma}}_{\text{SOC}}) + \tau_x \otimes (\Delta_0(\mathbf{p})\sigma_0 + \underbrace{\Delta_1 \cdot \boldsymbol{\sigma}}_{\text{triplet SC}})] \psi_{\mathbf{p}}$$

$$H_{\text{imp}} = \hat{U}(|\mathbf{r} - \mathbf{R}|) \tau_z \otimes \sigma_0 + \hat{J}(|\mathbf{r} - \mathbf{R}|) \tau_0 \otimes \mathbf{S} \cdot \boldsymbol{\sigma}$$

Let

$$G_{SC} \equiv [E - H_{SC}]^{-1}$$

Then the Schrodinger equation for the Hamiltonian  $H$  can be rewritten as  
(F. Pientka, L. I. Glazman, and F. von Oppen, PRB (2013))

$$\psi(\mathbf{p}) - G_{SC}(E, \mathbf{p}) \int_{\mathbf{p}'} H_{\text{imp}}(|\mathbf{p} - \mathbf{p}'|) \psi(\mathbf{p}') = 0.$$

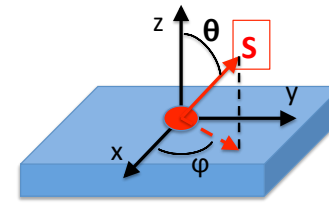
This equation admits nontrivial solutions for values of  $E$  such that

$$\det[1 - G_{SC}(E, \mathbf{p}) H_{\text{imp}}(|\mathbf{p} - \mathbf{p}'|)] = 0.$$

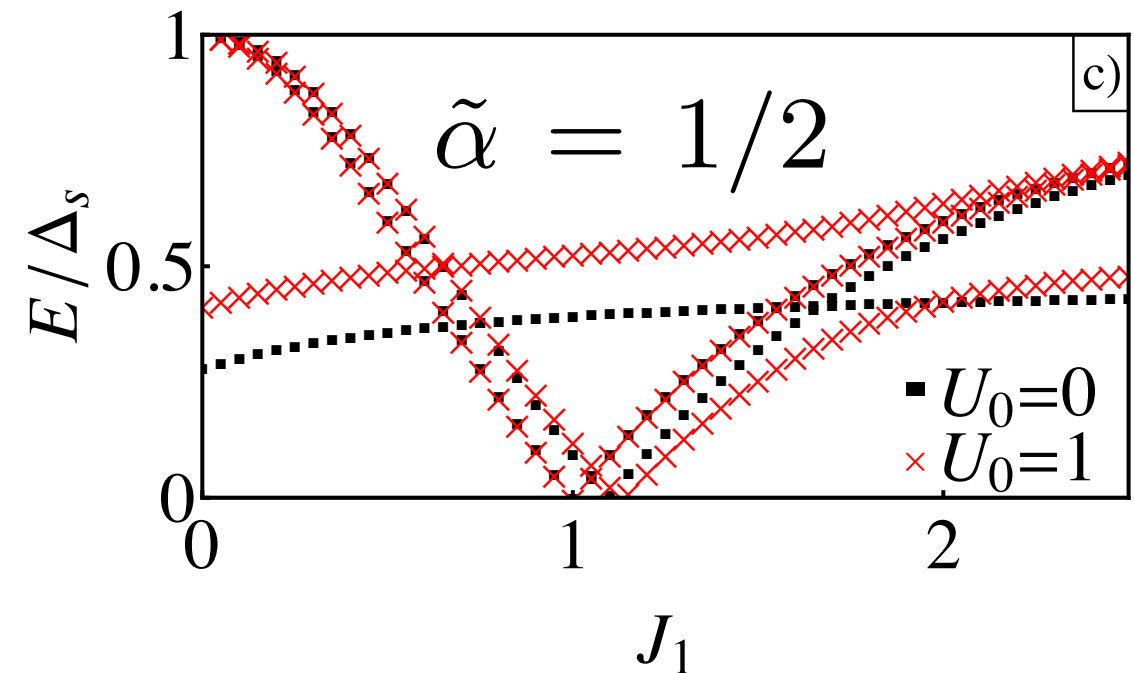
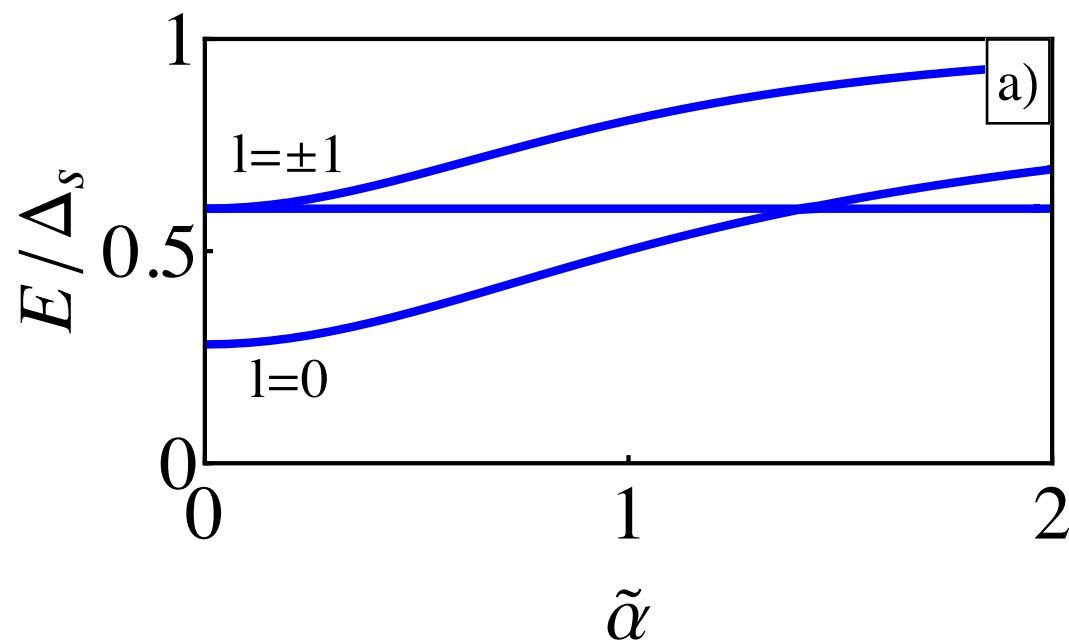
**For values of  $|E| < \Delta$  we have bound states (Shiba states)**

# Impurity-bound states in SCs with SOC: results

**s-wave superconductor**



$\theta=0$



$$\frac{|E_{l=0,1}|}{\Delta_s} = \frac{\gamma^2 - J_0^2 J_1^2 \pm \gamma^{\frac{3}{2}} \sqrt{(J_0^2 - J_1^2)^2 + (\gamma - 1)(J_0 - J_1)^4}}{\gamma^2(1 + (J_0 - J_1)^2) + 2\gamma J_0 J_1 + J_0^2 J_1^2}$$

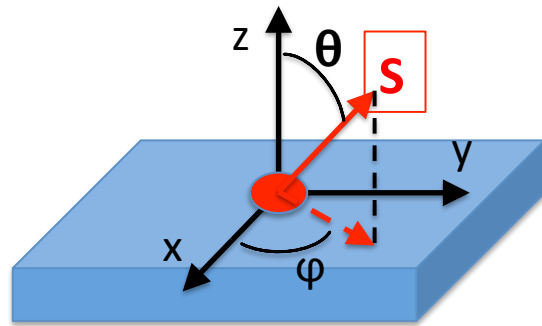
$$\gamma = 1 + \tilde{\alpha}^2$$

$$\frac{|E_{l=-1}|}{\Delta_s} = \frac{1 - J_1^2}{1 + J_1^2}$$

**As expected SOC mixes states with different  $l$ . It also causes an interplay of  $U$  and  $J$**

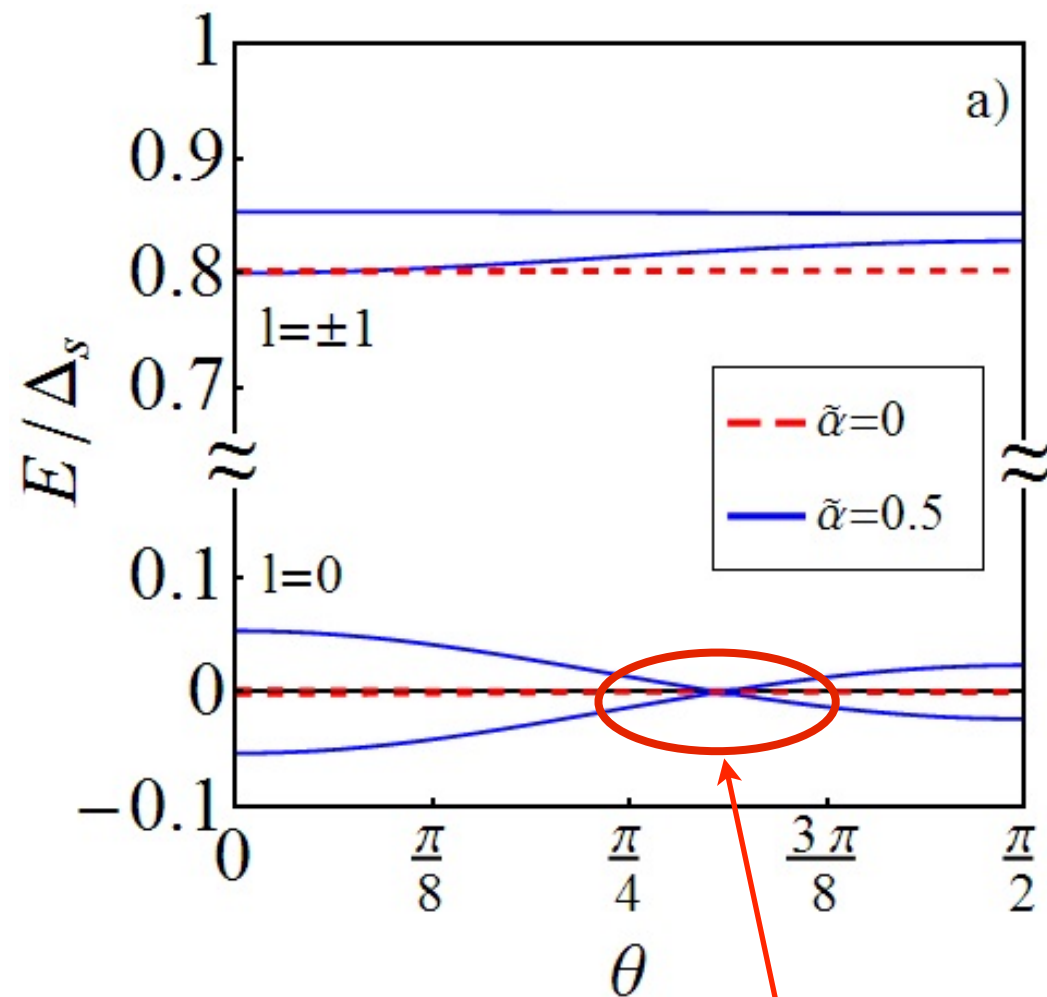
Y. Kim, J. Zhang, ER, R. Lutchyn  
arXiv:1410.4558 (2014)

# Impurity-bound states in SCs with SOC: results

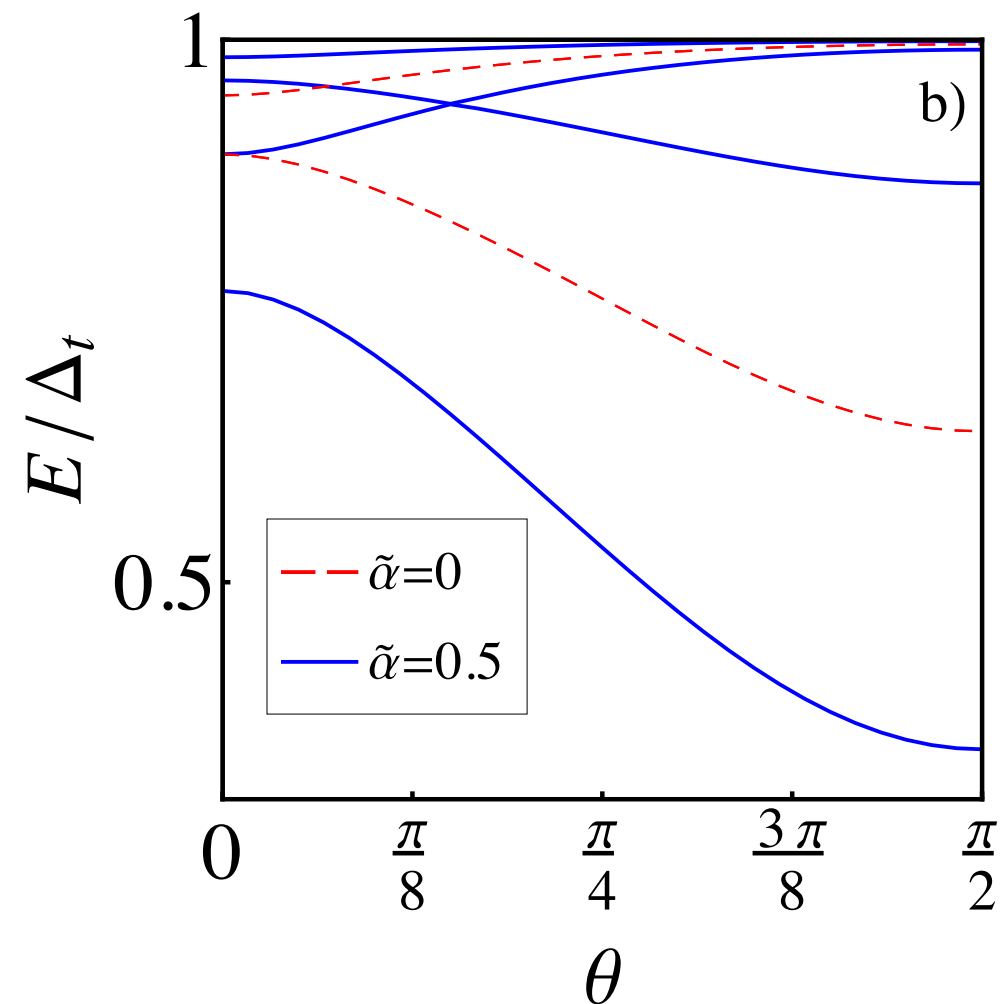


Dependence on  $\theta$

s-wave



p-wave



**SOC induces strong  $\theta$  dependence that can be used to tune the fermion parity of the bound state**

# Conclusions

- Obtained scaling of  $T_K$  and Kondo resistivity in 3D Dirac materials

$$\rho_K(T = 0) \propto \frac{n_{\text{imp}}}{n^{4/3}}$$

- Interplay of long-range disorder and Kondo effect in Dirac materials gives rise to a distribution of Kondo temperatures. Close to Dirac point:

$$P^{(3D)} \propto \frac{1}{T_K [\ln(T_K)]^{5/2}}$$

$$P^{(2D)} \propto \frac{1}{T_K [\ln(T_K)]^3}$$

- Low T tail of  $P(T_K)$  induces NFL

$$\chi_m \propto \frac{1}{T |\ln(T)|^{3/2}}$$

$$\chi_m \propto \frac{1}{T |\ln(T)|^2}$$

- Study effect of SOC on impurity bound states in 2D superconductors

SOC strongly affects the bound states created by isolated impurities in superconductors

Can change parity of Shiba state

# References

- A. Principi, G. Vignale, ER, arXiv 1410.8532 (2014)
- Y. Kim, J. Zhang, ER, R. Lutchyn, arXiv:1410.4558 (2014)

For more see:

<http://physics.wm.edu/~erossi/publications.html>